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LETTER TO THE EDITOR

Self-avoiding walks attached to triangular and face-centred cubic lattice surfaces: extended exact enumeration data

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Abstract. Analysis of exact enumeration data of self-avoiding walks attached to the surfaces of triangular and face-centred cubic lattices is consistent with $\gamma_1 = 0.718 \pm 0.008 + 136\,\Delta p_c$ where $\Delta p_c = p_c - 0.0995$, in three dimensions and $0.9530 \leqslant \gamma_1 \leqslant 0.9548$ in two dimensions, where p_c for the triangular lattice is assumed to lie in the range $0.240\,915 \leqslant p_c \leqslant 0.240\,93$.

In this letter we report on the analysis of extended exact enumeration data for self-avoiding walks (SAWs) attached to the surfaces of the semi-infinite triangular and face-centred cubic (FCC) lattices. (The semi-infinite FCC lattice is chosen to have a triangular lattice as its surface.) This work was motivated in part by the derivation of a possible exact result for the ordinary transition exponent γ_1 (Cardy 1984) in two dimensions and the increasing number of experimental results for surface critical phenomena in three-dimensional systems (for a list of these and a review of theoretical results see the article by Binder (1983)).

We have determined the first 14 terms for the triangular lattice and first 10 terms for the FCC lattice in the generating function

$$\chi_1 = \sum_n C_n p^n \underset{p \to p_c^-}{\sim} (p_c - p)^{-\gamma_1}(1 + \ldots) \tag{1}$$

where C_n is the number of n-step SAWs which start from a point on the surface (table 1) (γ_1 is the ordinary transition exponent).

Cardy (1984) has shown that assumptions about conformal invariance for two-dimensional systems at a phase transition lead to

$$\gamma_1 = 61/64. \tag{2}$$

A previous analysis of the first 10 terms in χ_1 for the triangular lattice was consistent with the above value of $\gamma_1(2)$ but had rather large error bounds and was based on biased Padé approximants at an assumed $p_c = 0.2408$ (De'Bell and Essam 1980). Analysis of the extended series supports a higher value of p_c and a revised estimate of γ_1, as detailed below. Cardy and Redner (1984) have analysed χ_1 for the square lattice using a ratio method and obtained a value of γ_1 consistent with (2). Guttmann

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Table 1. Coefficients c of the generating function $\chi_1 = \Sigma_n C_n p^n$ for SAWs originating at the surface of triangular and FCC lattices.

c (triangular)	c (FCC lattice)
1	1
4	9
16	81
66	753
272	7 143
1 118	68 403
4 160	658 959
19 018	6 377 829
78 514	61 962 261
324 330	603 845 955
1 340 338	
5 541 266	
22 916 110	
94 795 900	

and Torrie (1984) also argued that the above results for γ_1 should be exact and analysed the problem of a SAW in a wedge geometry in considerable detail.

Initially Padé approximants were formed to the logarithmic derivative of χ_1 for the triangular lattice. The poles of the higher-order approximants fall mainly in the range $0.2409 \leqslant p_c \leqslant 0.2410$ with a slight downward apparent trend and points on a pole-residue plot (apparently) falling on a smooth curve. Values of γ_1 obtained from this curve are consistent with (2) if we accept a value of $p_c \simeq 0.240\,89$, which is consistent with the downward trend seen in the Padé approximant estimates. (A similar analysis for walks in the bulk by Watts (1975) gave $p_c = 0.240\,85^{+0.000\,05}_{-0.000\,07}$).

In recent years, the importance of non-analytic 'corrections to scaling', represented by . . . in (1), in determining the exponent of the leading-order term have been demonstrated by a number of authors (Adler *et al* 1983 and references therein). Therefore, we have reanalysed χ_1 using the confluent singularity analysis described by Baker and Hunter (1973). In this analysis an auxiliary function is formed from χ_1, which has a simple pole at $1/\gamma_1$ and the position of this pole is estimated from Padé approximants to the auxiliary function.

Since the construction of the auxiliary function in the Baker-Hunter analysis requires the value of p_c as input, we performed the analysis for a number of trial values of p_c in the range $0.240\,86 \leqslant p_c \leqslant 0.240\,98$. The corresponding spread in the estimates of $1/\gamma_1$ is shown in figure 1. For trial values of p_c less than 0.240 915 the Padé approximants are not well converged; however, as this value of p_c is approached, the convergence rapidly improves and a region of best convergence is found for $0.240\,915 \leqslant p_c \leqslant 0.240\,93$. Assuming $p_c = 0.240\,915$ implies $\gamma_1 = 0.9537 \pm 0.0007$ in good agreement with the value obtained by Cardy (1984). However, the central estimate of γ_1 increases as the assumed value of p_c is increased so that assuming $p_c = 0.240\,92$ leads to $\gamma_1 = 0.9542 \pm 0.0006$, which is just inconsistent with the value obtained by Cardy. In short, while our results are consistent with $p_c = 0.240\,915$ and the proposed exact value of $\gamma_1(2)$, we cannot rule out a slightly higher value of p_c and subsequent small inconsistency with the proposed exact value for γ_1. As a further check on the consistency of our results with the proposed exact results when $p_c = 0.240\,915$, we have estimated $\gamma_{11} + 2\nu$

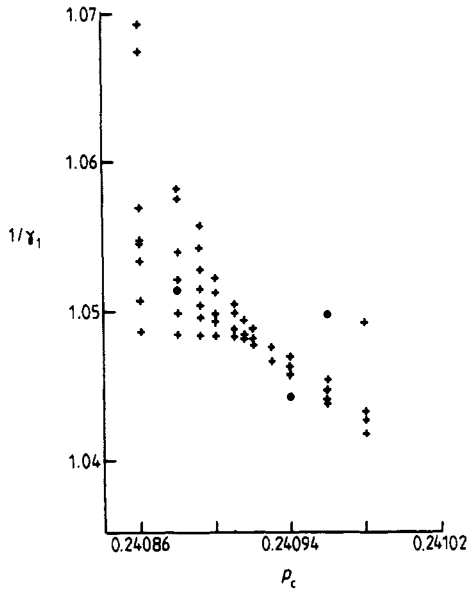

Figure 1. Location of the poles in the Padé approximants to the auxiliary function to the series χ_1 for the triangular lattice, formed by the Baker-Hunter (1973) method. The approximants shown are [6/4], [5/5], [6/5], [4/6], [6/6], [7/5], [7/6] and [5/7]. The [5/6] and [6/7] approximants have anomalous behaviour (e.g. regions with no physical pole) in this range of assumed p_c.

from the first nine terms of

$$\chi_{11}^{(2)} = \sum_n \sum_r C_n(\boldsymbol{r}) p_n r^2 \sim |p_c - p|^{-\gamma_{11} - 2\nu} \tag{3}$$

using the Baker-Hunter method for this value of p_c. $\chi_{11}^{(2)}$ was previously analysed by De'Bell and Essam (1980) by biased Dlog Padé approximants with $p_c = 0.2408$. In (3) $C_n(\boldsymbol{r})$ is the number of n-step walks from the origin to a site at $\boldsymbol{r}$ in the surface. Despite the small number of coefficients in $\chi_{11}^{(2)}$ available, the approximants are well converged and consistent with

$$\gamma_{11} + 2\nu = 1.323 \pm 0.013. \tag{4}$$

The scaling relation

$$2\gamma_1 - \gamma_{11} = \gamma + \nu \tag{5}$$

combined with the values of $\gamma_1 = 61/64$, $\nu = 3/4$, $\gamma = 43/32$ obtained from conformal invariance (Cardy 1984 and references therein) implies

$$\gamma_1 + 2\nu = 1.3125 \tag{6}$$

in good agreement with (4).

In the case of the FCC lattice, we again formed Padé approximants to the derivative of the logarithm of χ_1. The resulting pole-residue plot is shown in figure 2 and from this we obtain

$$\gamma_1 = 0.718 \pm 0.008 + 136\,\Delta p_c \tag{7}$$

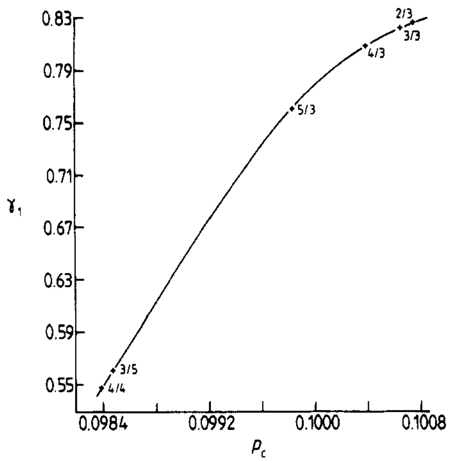

Figure 2. Pole-residue plot of Padé approximants to the derivative of the logarithm of χ_1 for the FCC lattice.

where the central estimate is for $p_c = 0.0995$ (De'Bell and Essam 1980) and the dependence on Δp $(= p_c - 0.0995)$ is estimated from the tangent at this point. Assuming $p_c = 0.0995$, the above estimate of $\gamma_1(7)$ is consistent with that obtained by other workers from exact enumeration data (0.70 ± 0.02 Barber *et al* 1978, Ishinabe and Whittington 1981) but inconsistent with the narrower range $0.675 \leq \gamma_1 \leq 0.680$ obtained by Eisenriegler *et al* (1982) from a Monte Carlo analysis for the tetrahedral lattice. Padé approximants to the auxiliary function generated by the Baker-Hunter analysis were not well converged for the FCC lattice; however, it seems probable that the uncertainty in γ_1, due to the small number of terms available and uncertainty in p_c, is relatively large compared with the more subtle effects of correction to scaling terms.

In summary, analysis of exact enumeration data for SAWS attached to a surface results in the estimates of γ_1 (for the ordinary transition) for the triangular and FCC lattice quoted in the abstract. In the case of the triangular lattice, we have used the method of Baker and Hunter (1973) to allow for confluent singularities and the best convergence of the Padé approximants occurs for trial values of the critical value of p in the range $0.240\,915 \leq p_c \leq 0.240\,93$. Our results are consistent with the value of $\gamma_1 = 64/61$ obtained by Cardy (1984) only at the lower extreme of this range of values for p_c. The range of values for γ_1 quoted in the abstract represents only the total variation in the Padé approximants in this range of p_c and, we emphasise, is not an absolute measure of the uncertainty in γ_1. Our analysis of the FCC lattice data has been limited to a conventional Dlog Padé analysis and the estimate of γ_1 in the abstract was read from the corresponding pole-residue plot (figure 2). Notice that the estimate of γ_1 is strongly dependent on the value of p_c for the FCC lattice.

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